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Accelerating the Commercialization of CCS Technology**

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INTRODUCTION

The *Carbon Capture Simulation Initiative* (CCSI) is a partnership among national laboratories, industry and academic institutions that will develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. The *CCSI Toolset* will provide end users in industry with a comprehensive, integrated suite of scientifically validated models with uncertainty quantification, optimization, risk analysis and decision making capabilities. The CCSI Toolset will incorporate commercial and open-source software currently in use by industry and will also develop new software tools as necessary to fill technology gaps identified during execution of the project. The CCSI Toolset will (1) enable promising concepts to be more quickly identified through rapid computational screening of devices and processes; (2) reduce the time to design and troubleshoot new devices and processes; (3) quantify the technical risk in taking technology from laboratory-scale to commercial-scale; and (4) stabilize deployment costs more quickly by replacing some of the physical operational tests with a virtual power plant.

CCSI will leverage DOE/NETL's comprehensive CCS RD&D program, part of the President's plan to overcome the barriers to the widespread, cost-effective deployment of CCS within 10 years (Presidential Memo, 2010). It has been estimated that using today's commercially available CCS technologies would add approximately 80 percent to the cost of electricity for a new pulverized coal (PC) plant and approximately 35 percent to the cost of electricity for a new advanced gasification-based plant. Thus, an important part of the CCS RD&D effort is the development of the next generation of technologies for carbon capture that have the potential to reduce these costs to less than a 30 percent increase in the cost of electricity for PC power plants and less than a 10 percent increase in the cost of electricity for new gasification-based power plants (Ciferno et al. 2010). For PC plants, the majority of the increased costs result from the parasitic loads (steam and power) required for the CO₂ capture and compression processes, which decrease the power generating efficiency (and the net output) by approximately one third.

Taking promising new power plant technologies from concept to commercial scale could take 20-30 years because of the need to manage the overall risk of the scale-up process. Typically, several incremental steps are taken during scale-up, ensuring that the risk in each step is as small as possible. The CCSI will provide validated simulation tools that will accelerate the commercial deployment technologies developed under the CCS RD&D program. Science-based models will be used in conjunction with pilot-scale data to allow larger steps to be taken earlier with greater confidence, thereby reducing the time and expense required for achieving commercial deployment of carbon capture technology.

Recent experience in other industries such as aerospace and the automotive industry has demonstrated that simulations can be used to accelerate the development of technology (Schrage, 2000; NRC, 2002; Koonin, 2010). The challenge addressed by CCSI is to use the recent advances in simulation technology and to develop a science-based capability to assess and mitigate the risk of scaling up carbon capture technologies.

INDUSTRY CHALLENGE PROBLEMS

The CCSI Toolset will be developed by focusing on three industrial challenge problems (ICP). It is particularly important to develop capabilities that can address the largest potential sources of CO₂. For this reason, the initial CCSI effort will focus on methods applicable to PC power plants, which generate nearly half the electricity in the United States, and emit about a third of all CO₂ from U.S. sources. Ninety-five percent of the coal-based CO₂ emissions projected to be released from 2010 through 2030 will originate from existing PC power plants. A recent analysis suggests that roughly 325 coal-fired generating units accounting for roughly two thirds (200 GW) of current U.S. coal-based generating capacity are suitable for carbon capture (Nichols, 2010).

Solid-sorbent-based post-combustion capture (ICP A)

Solid-sorbent-based post-combustion capture technology was chosen as the first ICP for CCSI because, while DOE/NETL is sponsoring a number of sorbent development efforts, significant work remains to define and optimize the reactors and processes needed for successful sorbent capture systems. Sorbents offer an advantage because they can reduce the regeneration energy associated with CO₂ capture, thus reducing the parasitic load. Most of the work on sorbents has been restricted to developing the sorbent itself (Sjostrom and Krutka, 2010) with only very recent studies considering the design of the reactor system and integration with the power plant (Sjostrom, 2010). Thus, *solid-sorbent systems are at the start of the traditional process development cycle*. An ICP focused on solid sorbents will accelerate the analysis of options for this emerging technology. The CCSI Toolset will help identify promising solid-sorbent processes and accelerate the scale-up from 25 MWe to commercial demonstration scales.

Solvent based post-combustion capture (ICP B)

Solvent-based post-combustion capture was chosen as the second ICP because it is quite likely that solvent scrubbing will be deployed by industry as a CCS technology. Commercial solvent developers have already completed process design and analysis for first generation solvents, and these are being tested in various pilots. Because of the significant commercial practice that already exists for commercial amine solvents, it is recognized that any near-term CCSI developments would be secondary to empirical knowledge or optimization that has already been practiced. In contrast, *advanced solvents are currently in the middle of the traditional process development cycle*, moving from pilot scale to commercial demonstration, so CCSI development can build logically on the prior developments for solid sorbents, chronologically matching current industrial development of advanced solvents. Experimental validation data for advanced solvents is expected from pilot tests now in progress or being planned (Maxwell, 2010). Such data from pilot testing of these existing solvents will be used to validate the CCSI Toolset, and provide confidence that these tools can be used in the future with advanced solvents. The CCSI Toolset will also enable consideration of process dynamics, such as load following, that are not typically explored with steady-state process flowsheets.

Oxy-combustion (ICP C)

Oxy-combustion was chosen as the third ICP because of the expected timelines for oxy-combustion pilot and demonstration projects. Validation data from these current projects will be used to gain confidence in the CCSI Toolset, which will then be used to extrapolate demonstration project designs to second generation configurations, operation on different coal types, and retrofit analysis for existing plants. In contrast to the first two ICPs, the oxy-combustion case will add progressively more complex analysis capabilities to the CCSI Toolset. It will require adding details of the plant configuration (e.g., boiler interior, fuel handling, air preheating) that are not needed to assess an “add-on” technology, such as addressed in the first two ICPs.

Oxy-combustion is different from the first two ICPs in that it requires modifying the boiler and auxiliary systems to provide oxygen, recycle flue gas, and flue gas purification after water vapor condensation. A key aspect for efficient operation is integration of heat from the air separation plant, the CO₂ compressors, and gas purification unit. Improved integration of these subsystems has been reported from commercial developers. This is expected to reduce the efficiency penalty of oxy-combustion relative to current post-combustion capture with amine solvents.

Oxy-combustion development has progressed significantly in the last decade. A 30MWth pilot plant is already operating in Schwarze Pumpe, Germany, and several other demonstration plants are planned or being developed, including the U.S. DOE FutureGen 2.0 plant (FutureGen, 2010), as well as other demonstrations summarized by Wall and Yu (2009). These demonstrations will offer a valuable platform to validate the CCSI Toolset and subsequently to apply the tools for wider commercial deployment of oxy-combustion technology. Since current generation of *oxy-combustion systems is near the end of the traditional process development cycle*, the CCSI Toolset development will be available to consider design improvements, adaptations to handle different coal types, new approaches to oxygen generation, advanced cooling towers (e.g., air cooling, wet surface, etc.), as well as evaluate process dynamics.

CROSS-CUTTING CHALLENGES

Some of the challenges that the ICPs address will be specific to a given CCS technology (e.g., the ability to correctly simulate the rate and impacts of attrition of a particular solid sorbent in a large-scale system, or the performance of a large-scale absorber using an advanced liquid solvent). Other challenges will be common to all systems, such as the integration of component models, the prediction of dynamic behavior, the impact of trace impurities, or the potential for corrosion/erosion of vessels, ductwork or equipment. The strength of our ICP approach is that it will advance the state of the art by focusing on one concrete application at a time, identifying and resolving all the critical issues that must be resolved in order to confidently scale-up that class of technology, while developing a common simulation framework, common data management, and common software components that can be reused or extended to simulate other carbon capture technologies.

In building a common framework and reusable/extendable components, CCSI will adhere to modern software design principles and incorporate state-of-the-art modeling and simulation technologies. Specific challenges that will be addressed include the following:

A consistent data set and model verification and validation (V&V) hierarchy. The CCSI Toolset will ensure that all the simulations within its framework use consistent data formats (e.g., the same thermo-physical properties are used in models at various scales) with assured data provenance. A model V&V hierarchy will be built to validate models at different scales (e.g., sorbent pellet, absorber column, capture process, capture process integrated with power plant) that constitute the virtual power plant with carbon capture.

Integrated models. The CCSI Toolset will ensure the consistency of models across all length scales. Thus, knowledge gained from models at any scale will be preserved when decisions are being made with models at other scales. Absent our approach, ensuring model consistency is a time consuming process involving scientists and engineers from different disciplines and institutions who often lack a common understanding of the goals and limitations of models at other scales. In addition, complex lower length scale models when used in a larger length scale model could make the integrated model computationally intractable. CCSI will develop a common platform that allows models to readily exchange information in a computationally efficient manner, enabling the development of complete (knowledge preserving) and consistent models.

Uncertainty quantification. Model predictions contain uncertainties that result from several sources including: (a) uncertainties in basic input data (e.g., material properties or chemical reaction rates); (b) uncertainties in the output of one model that is used as the input to another model; (c) uncertainties that arise when a model validated at a certain scale is used for simulations at a larger scale; and (d) uncertainties due to “unknown unknowns” such as unanticipated chemistries, flow patterns, or materials problems that are encountered for the first time when a process is scaled up. In addition to providing tools to quantify these uncertainties, CCSI will characterize uncertainties in terms of the risks involved in different levels of scale-up.

Optimization based on integrated models. Optimization tools are essential for decision making as they provide superior, consistent designs among practitioners with various levels of expertise, provide new insights to novel designs, and have been demonstrated to reduce the design cycle by one or two orders of magnitude. CCSI will address the challenge of optimizing large-scale integrated models with quantified uncertainties.

Risk analysis and decision making. CCSI will address the challenge of integrating risk analysis into the simulation framework so that information from science-based models is used to facilitate risk analysis and decision making.

TECHNICAL APPROACH

As shown in Table 1, the CCSI team has been organized into three focus areas and ten Task Sets (TS) to address the challenges in multi-scale and multi-physics modeling and analysis, software implementation, and industrial applications.

Table 1 CCSI Task Sets by Focus Area

Physicochemical Models and Data	Analysis & Software	Industrial Applications
1. Basic Data and Models	5. Integration Framework	9. Industrial Challenge Problems
2. Particle and Device Scale Models	6. Uncertainty Quantification	10. Industrial Collaboration
3. Process Synthesis and Design	7. Risk Analysis and Decision Making	
4. Plant Operations and Control	8. Software Development Support	

The *Physicochemical Models and Data* focus area consists of four TSs that address the challenge of developing science-based modeling tools for various CCS processes considered in the ICPs. The models range from particle scale reaction kinetics models, to device scale CFD models, to steady-state process synthesis and design models, to dynamic plant operations and control models. A parallel top down (i.e., starting with full scale) and bottom up (i.e., starting with small scale) approach will be pursued. The top down approach will help to identify and evaluate the equipment and system configurations that will ultimately be required to put the technology into practice. The bottom up approach, which mimics current practice of multiple scale ups from laboratory to pilot to intermediate scale, will provide a rigorous framework for developing the required fundamental models. The top down approach will also help identify key aspects of the fundamental models that have the highest projected impact on overall plant performance. Several commonly used commercial and open-source software such as FLUENT[®], Aspen Plus[®], DYNsIM[®], and MFiX will be used to build the models. Unlike other modeling efforts, the simulation and design activities at the different length scales (e.g., CFD and process system) will be integrated so that information and insight will continually flow between scales so that each scale can benefit from insights at the other scales. Much of this information flow will result from an integration framework being built by the second focus area.

The *Analysis & Software* focus area includes four TSs that will develop the capability to integrate different models and software packages, to quantify uncertainties in model predictions, to develop optimal designs based on integrated models, and to conduct risk analysis. An additional TS will support software development across all the TSs. Realizing the vision of an integrated and coherent multi-scale software environment for the design, analysis, and optimization of carbon capture systems requires an approach that effectively enables the flow of information between the scales of interest. This capability will be largely data-driven, and performance at varying operating conditions will require proper data management, reuse and tracking. An archival system is required with support for the derivation, reuse and performance monitoring at different levels of

scale to enable key decision-support capabilities. In addition to technical risks, the development and deployment of new technology poses various economic and legal risks. Modeling and simulation can address some of the technical and economic risks through the use of predictive computer models, if the uncertainties inherent in the modeling process can be determined. Uncertainties that need to be addressed are related to the data used to describe the physicochemical models, coupling the results of one simulator to another, and in the extrapolation into poorly known regions of parameter space needed to explore new design scenarios. The assessment of economic and legal risks is only possible if a well defined process is in place for assessing the propagation of uncertainties, sensitivity analysis, model reduction, model validation and calibration, and risk analysis of large-scale multi-physics technical models.

The *Industrial Applications* focus area consists of two TS's: Industrial Challenge Problems and Industrial Collaboration. CCSI's industry partnerships are of critical value to the project's success. The Industrial Collaboration TS is responsible for developing a strong collaboration between the industry partners and other CCSI partners and for ensuring that CCSI models are applied to support commercial decisions that will accelerate capture deployment. It will also facilitate the full utilization of data from industry demonstration facilities to support CCSI plant level models without compromising the competitive position of commercial partners. The Industrial Challenge Problems TS is responsible for working with the industry partners to develop and refine the three ICPs. It will also be responsible for evaluation of the CCSI Toolset and results from its application. The ultimate objective of accelerating the deployment of capture technology requires that the tools and methodologies developed provide information necessary to support investment decisions by equipment suppliers and utility companies. Our industry partners will help ensure that CCSI understands these information requirements and can communicate simulation results in a manner appropriate to aid decision makers.

SUMMARY

Over five years, CCSI will develop an integrated, validated suite of models and computational tools for accelerating the development and deployment of carbon capture technology. The CCSI Toolset will be used during the scale-up of carbon capture processes to assess and mitigate technical and financial risks, to improve designs, and to shorten the design cycle. This will support decision making to move to larger scales, more quickly and with better designs, thereby considerably reducing the cost and time required for the commercialization of carbon capture technology.

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